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=> d que sta l13 L11 STR

P---- C---- P 1 2 3 4

NODE ATTRIBUTES:

NSPEC IS R AT 1 NSPEC IS R AT 4 DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 4

STEREO ATTRIBUTES: NONE

L13 179 SEA FILE=REGISTRY SSS FUL L11

100.0% PROCESSED 81481 ITERATIONS

SEARCH TIME: 00.00.01

179 ANSWERS

=> b hcap FILE 'HCAPLUS' ENTERED AT 16:11:09 ON 10 AUG 2006 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 10 Aug 2006 VOL 145 ISS 7
FILE LAST UPDATED: 9 Aug 2006 (20060809/ED)

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 This file contains CAS Registry Numbers for easy and accurate
 substance identification.
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     ANSWER (1 OF 3 ) HCAPLUS COPYRIGHT 2006 ACS on STN
L33
                   HCAPLUS
AN
     2004:287803
DN
     140:310272
     Entered STN: 08 Apr 2004
ED
     Process for the hydroformylation of an ethylenically unsaturated compound
TI
IN
     Drent, Eit; Van Ginkel, Roelof; Jager, Willem
     Shell Internationale Research Maatschappij B.V., Neth.
PA
so
     PCT Int. Appl., 28 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
IC
     ICM B01J-0031/24
          B01J-0027/08; B01J-0031/02; C07F-0009/6568; C07F-0015/00;
           C07C-0045/50
     67-1 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
CC
     Section cross-reference(s): 23
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                                                APPLICATION NO.
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              OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
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CLASS
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 WO 2004028689
                  ICM
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                  ICS
                          B01J-0027/08; B01J-0031/02; C07F-0009/6568;
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                         B01J0031-24 [I,A]; C07C0045-00 [I,C*]; C07C0045-50 [I,A]; C07F0009-00 [I,C*]; C07F0009-6568 [I,A];
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                         4G169/BC69A; 4G169/BC72A; 4G169/BC72B; 4G169/BE26A;
                         4G169/BE26B; 4G169/BE37A; 4G169/BE37B; 4G169/CB51;
                         4G169/FA01; 4H006/AA02; 4H006/AC48; 4H006/BA25;
                         4H006/BA35; 4H006/BA44; 4H006/BA47; 4H006/BA81;
                         4H006/BE20; 4H006/BE40; 4H006/BN10; 4H006/BT12;
                         4H039/CC30; 4H039/CL45
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ECLA

[I,A]; C07C0067-347 [I,A]; C07F0009-6568 [I,A]

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B01J031/24; C07C045/50; C07C067/347+69/675;
                        C07C067/347+69/716; C07F009/6568C
os
     MARPAT 140:310272
     The present invention relates to a process for the hydroformylation of an
AB
     optionally substituted ethylenically unsatd. compound by reaction thereof
     with carbon monoxide and hydrogen in the presence of a specific catalyst
     system. The specific catalyst system comprises (A) a source of group VIII
     metal cations, (B) a diphosphine ligand having the general formula X1RX2,
     (C) an acid with pKa < 3, measured in an aqueous solution at 18^{\circ} or a salt
     derived thereof, and (D) a source of halide anions, wherein X1, X2 =
     independently an optionally substituted cyclic group with ≥5 ring
     atoms, of which one is a phosphorus atom, and R = a bivalent optionally
     substituted bridging group, connected to each phosphorus atom by a sp2
     hybridized carbon atom. Furthermore some specific bidentate diphosphines
     used in this process are described. Thus, 1,2-dibromobenzene 9.44,
     1,4-diazabicyclo[2,2,2]octane 22.4, 9-phosphabicyclo[3.3.1]nonane 13.0,
     and tetrakis(triphenylphosphine)palladium 2.32 g were heated at
     140° to give 7.10 g (yield 50%) 1,2-bis(9-
     phosphabicyclo[3.3.1]nonyl)benzene, 0.40 mmol of which was mixed with
     methane sulfonic acid 1.0, hydrochloric acid 0.20, and palladium acetate
     0.25 mmol, and 20 mL 1-octene and heated at 120° for 5 h under 20
     bar carbon monoxide and 40 bar hydrogen to give an alkanol product >99, a
     linear alkanol product 68, and a hydrogenation product <1%.
     process hydroformylation ethylenically unsatd compd;
     bisphosphabicyclononylbenzene ligand palladium acetate catalyst octene
     hydroformylation
IT
     Alkenes, reactions
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (C11-12; hydroformylation of ethylenically unsatd. compds.)
IT
     Ligands
     RL: CAT (Catalyst use); USES (Uses)
        (bidentate, diphosphines, hydroformylation catalyst
        ligand; hydroformylation of ethylenically unsatd. compds.)
IT
     Hydroformylation
        (hydroformylation of ethylenically unsatd. compds.)
IT
     Group VIII elements
     RL: CAT (Catalyst use); USES (Uses)
        (hydroformylation of ethylenically unsatd. compds.)
IT
     Catalvsts
        (hydroformylation; hydroformylation of ethylenically unsatd. compds.)
IT
     676992-18-0 676992-19-1
     RL: CAT (Catalyst use); USES (Uses)
        (hydroformylation catalyst ligand; hydroformylation of ethylenically
        unsatd. compds.)
IT
     407578-79-4P, 9-Phosphabicyclo[3.3.1] nonane, 9,9'-(1,2-
     phenylene)bis- 676992-15-7P
                                  676992-16-8P
     RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation);
    USES (Uses)
        (hydroformylation catalyst ligand; hydroformylation of ethylenically
        unsatd. compds.)
IT
     3375-31-3
     RL: CAT (Catalyst use); USES (Uses)
        (hydroformylation of ethylenically unsatd. compds.)
IT
     4547-43-7P, Hexanoic acid, 6-hydroxy-, methyl ester 167707-57-5P,
     Pentanoic acid, 5-hydroxy-4-methyl-, methyl ester
                                                         676992-17-9P
     RL: IMF (Industrial manufacture); PREP (Preparation)
        (hydroformylation of ethylenically unsatd. compds.)
    111-66-0, 1-Octene
                        630-08-0, Carbon monoxide, reactions
     818-59-7
               1333-74-0, Hydrogen, reactions
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (hydroformylation of ethylenically unsatd. compds.)
IT
     583-53-9, 1,2-Dibromobenzene
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     13887-02-0, 9-Phosphabicyclo[3.3.1] nonane
                                                 75415-78-0,
     1,2-Dibromocyclopentene
     RL: RCT (Reactant); RACT (Reactant or reagent)
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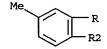
(reactant in hydroformylation catalyst ligand preparation; hydroformylation of ethylenically unsatd. compds.)

676992-18-0 IT

RL: RCT (Reactant); RACT (Reactant or reagent) (hydroformylation catalyst ligand; hydroformylation of ethylenically unsatd. compds.)

RN 676992-18-0 HCAPLUS

CN 9-Phosphabicyclo[3.3.1]nonane, 9,9'-(4-methyl-1,2-phenylene)bis- (9CI) (CA INDEX NAME)







ANSWER (2 OF 3) HCAPLUS COPYRIGHT 2006 ACS on STN L33

HCAPLUS ΑN 2002:295834

DN 137:108974

Entered STN: 21 Apr 2002 ED

Teaching a palladium polymerization catalyst to mono-oxygenate olefins TT

MILLICATE

Drent, E.; Mul, W. P.; Budzelaar, P. H. M. ΑU

Shell Research and Technology Centre, Amsterdam, Amsterdam, Neth. CS

Comments on Inorganic Chemistry (2002), 23(2), 127-147 SO CODEN: COICDZ; ISSN: 0260-3594

PB Taylor & Francis Ltd.

Journal DT

LА English

22-7 (Physical Organic Chemistry) CC Section cross-reference(s): 51, 67

CASREACT 137:108974 OS AB

Catalyst systems consisting of a palladium(II) diphosphine complex with weakly or non-coordinating counterions are efficient catalysts for the hydrocarbonylation of olefins. With these catalyst systems, the oxo-synthesis can be fully exploited to produce, at will, aldehydes/alcs. by hydroformylation or monoketones by hydro-acylation of olefins. The reactions described here constitute the first examples of selective formation of ketones by hydrocarbonylation of higher olefins and the first examples of Pd catalyzed hydroformylation of olefins. Variation of ligand, anion and/or solvent can be used to steer the reaction selectively towards aldehydes/ alcs., ketones or oligoketones. Non-coordinating anions and arylphosphine ligands produce primarily (oligo)ketones; increasing ligand basicity shifts selectivity towards monoketones, while increasing ligand basicity and/or increasing anion coordination strength leads to high selectivity for hydroformylation products, aldehydes and alcs. For the mechanisms of the aldehyde-producing step, we propose protonation of Pd(II)-acyl intermediates, assisted by the coordination of the anion, followed by reductive elimination of the aldehyde and heterolytic dihydrogen cleavage. For selective saturated monoketone formation we propose protonation at the Pd(II)-alkyl stage, now assisted by

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chelating carbonyl coordination followed by reductive elimination of the ketone and heterolytic dihydrogen cleavage. Unsatd. ketone formation involves β-hydride elimination from the same Pd(II)-alkyl intermediates. olefin hydrocarbonylation hydroformylation palladium catalyst Ligands RL: CAT (Catalyst use); USES (Uses) (bidentate phosphines; hydrocarbonylation of olefins using catalyst systems consisting of a palladium(II) diphosphine complex with weakly or non-coordinating counterions) Alcohols, preparation RL: SPN (Synthetic preparation); PREP (Preparation) (formation under hydroformylation conditions; hydrocarbonylation of olefins using catalyst systems consisting of a palladium(II) diphosphine complex with weakly or non-coordinating counterions) Addition reaction Hydroaddition reaction catalysts (hydroacylation; hydrocarbonylation of olefins using catalyst systems consisting of a palladium(II) diphosphine complex with weakly or non-coordinating counterions) Hydroformylation Hydroformylation catalysts Regiochemistry Solvent effect (hydrocarbonylation of olefins using catalyst systems consisting of a palladium(II) diphosphine complex with weakly or non-coordinating counterions) Alkenes, reactions RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or (hydrocarbonylation of olefins using catalyst systems consisting of a palladium(II) diphosphine complex with weakly or non-coordinating counterions) Aldehydes, preparation Ketones, preparation RL: SPN (Synthetic preparation); PREP (Preparation) (hydrocarbonylation of olefins using catalyst systems consisting of a palladium(II) diphosphine complex with weakly or non-coordinating counterions) Chemoselectivity (hydroformylation vs. hydroacylation; hydrocarbonylation of olefins using catalyst systems consisting of a palladium(II) diphosphine complex with weakly or non-coordinating counterions) Anions (ligand/anion effects on catalysis; hydrocarbonylation of olefins using catalyst systems consisting of a palladium(II) diphosphine complex with weakly or non-coordinating counterions) Steric effects (of phosphine ligand; hydrocarbonylation of olefins using catalyst systems consisting of a palladium(II) diphosphine complex with weakly or non-coordinating counterions) Carbonylation Carbonylation catalysts (reductive; hydrocarbonylation of olefins using catalyst systems consisting of a palladium(II) diphosphine complex with weakly or non-coordinating counterions) Synthesis gas (selective production of ketones or aldehydes at will from olefins and syngas; hydrocarbonylation of olefins using catalyst systems consisting of a palladium(II) diphosphine complex with weakly or non-coordinating counterions) Ketones, preparation RL: SPN (Synthetic preparation); PREP (Preparation) $(\alpha, \beta$ -unsatd.; hydrocarbonylation of olefins using catalyst

systems consisting of a palladium(II) diphosphine complex with weakly

```
or non-coordinating counterions)
     76-05-1, Trifluoroacetic acid, uses
                                             104-15-4, p-Toluenesulfonic acid,
IT
           1493-13-6, Trifluoromethanesulfonic acid
     RL: CAT (Catalyst use); USES (Uses)
        (anion precursor; hydrocarbonylation of olefins using catalyst systems
        consisting of a palladium(II) diphosphine complex with weakly or
        non-coordinating counterions)
     3375-31-3, Palladium diacetate
TΤ
     RL: CAT (Catalyst use); USES (Uses) (catalyst precursor; hydrocarbonylation of olefins using catalyst
        systems consisting of a palladium(II) diphosphine complex with weakly
        or non-coordinating counterions)
                                    7786-29-0P, \alpha-Methyloctanal
IT
     78-84-2P, Isobutyraldehyde
     27644-47-9P, \alpha-Propylhexanal 27649-40-7P, \alpha-Ethylheptanal
     RL: BYP (Byproduct); PREP (Preparation) (hydrocarbonylation of olefins using catalyst systems consisting of a
        palladium(II) diphosphine complex with weakly or non-coordinating
        counterions)
     111-66-0, 1-Octene 115-07-1, Propene, reactions
IT
     RL: CPS (Chemical process); PEP (Physical, engineering or chemical
     process); RCT (Reactant); PROC (Process); RACT (Reactant or
         (hydrocarbonylation of olefins using catalyst systems consisting of a
        palladium(II) diphosphine complex with weakly or non-coordinating
        counterions)
                                                  7379-12-6P, 2-Methyl-3-hexanone
IT
     123-72-8P, Butanal
                           124-19-6P, Nonanal
     53252-19-0P, 2-Methyl-4-hexen-3-one 62834-80-4P, 2-Methyl-1-hexen-3-one
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (hydrocarbonylation of olefins using catalyst systems consisting of a
        palladium(II) diphosphine complex with weakly or non-coordinating
        counterions)
     6737-42-4, 1,3-Bis(diphenylphosphino)propane
IT
                                                       121115-33-1,
                                                131285-34-2, 1,3-
     1,3-Bis(di-tert-butylphosphino)propane
     Bis (dibutylphosphino) propane 143540-35-6, 1,3-Bis (di-sec-
     butylphosphino) propane
                               159460-98-7, 1,2-Bis(di-sec-butylphosphino)ethane
     RL: CAT (Catalyst use); USES (Uses)
         (ligand; hydrocarbonylation of olefins using catalyst systems
         consisting of a palladium(II) diphosphine complex with weakly or
        non-coordinating counterions)
               THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE.CNT
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    Syntheses with Carbon Monoxide 1980
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     3375-31-3, Palladium diacetate
     RL: CAT (Catalyst use); USES (Uses); RCT (Reactant); RACT
      (Reactant or reagent)
         (catalyst precursor; hydrocarbonylation of olefins using catalyst
         systems consisting of a palladium(II) diphosphine complex with weakly
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lao 10 / 670105
        or non-coordinating counterions)
RN
     3375-31-3 HCAPLUS
     Acetic acid, palladium(2+) salt (8CI, 9CI) (CA INDEX NAME)
CN
    - CH CH3
●1/2 Pd(II)
    ANSWER (3 OF 3 HCAPLUS COPYRIGHT 2006 ACS on STN 2001:851170 HCAPLUS
L33
AN
DN
     135:371865
     Entered STN: 23 Nov 2001
     Bidentate ligands useful as carbonylation catalysts
тT
     Drent, Eit; Eberhard, Michael Rolf; Pringle, Paul Gerard
IN
     Shell Internationale Research Maatschappij BV, Neth.
PA
     PCT Int. Appl., 25 pp.
SO
     CODEN: PIXXD2
DT
     Patent
     English
LA
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     ICS C07F-0009/6568; C07F-0009/6571; C07C-0045/50; B01J-0031/24
     29-7 (Organometallic and Organometalloidal Compounds)
CC
     Section cross-reference(s): 45
FAN.CNT 1
     PATENT NO.
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                                DATE
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                                            ______
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                                          2001WO-EP05625
     WO2001087899
                                20011122
                        A1
DT
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DATE W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG 2001CA-2408862 20010516 CA---2408862 AA 20011122EP---1282629 2001EP-0940491 20010516 20030212 **A1** EP---1282629 B1 20040204 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR 20030610 2001BR-0010882 20010516 BR2001010882 Α 2001JP-0584292 20010516 JP2003533534 **T2** 20031111 20040215 2001AT-0940491 20010516 AT---258936 E 2001ES-1940491 20010516 ES---2210170 **T**3 20040701 2001US-0860015 20010517 US2002016484 **A1** 20020207 20031028 US---6639091 B2 2002ZA-0009309 20021115 ZA2002009309 Α 20030729 PRAI 2000EP-0304171 Α 20000517 20010516 2001WO-EP05625 W CLASS PATENT FAMILY CLASSIFICATION CODES PATENT NO. CLASS _____ WO 2001087899 ICM C07F-0009/50 C07F-0009/6568; C07F-0009/6571; C07C-0045/50; ICS B01J-0031/24 C07F0009-50 [ICM, 7]; C07F0009-6568 [ICS, 7]; IPCI C07F0009-6571 [ICS,7]; C07F0009-00 [ICS,7,C*]; C07C0045-50 [ICS,7]; C07C0045-00 [ICS,7,C*];

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                         C07F009/50A6; C07F009/6568C; C07F009/6571L
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                 IPCI  BOIJ [ICM,7]; CO7C [ICS,7]; CO7F [ICS,7]
     CASREACT 135:371865; MARPAT 135:371865
os
AB
     The invention describes bidentate ligands of formula R1R2M1-R-M2R3R4,
     wherein M1 and M2 are independently P, As or Sb; R1, R2, R3 and R4
     independently represent tertiary alkyl groups, or R1 and R2 together
     and/or R3 and R4 together represent an optionally substituted bivalent
     cycloaliph. group whereby the two free valencies are linked to M1 or M2,
     and R represents a bivalent aliphatic bridging group containing from 2 to 6 atoms
     in the bridge, which is substituted with two or more substituents. Use of
     such a catalyst system in a process for the carbonylation of optionally
     substituted alkenes and alkynes by reaction with carbon monoxide and a
     coreactant is described. Thus, propene is hydroformylated by
     pressurization with carbon monoxide and hydrogen in the presence of
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platinum(II) acetylacetonate and meso (R,S) 2,3-
     [bis(cyclooctylenephosphino)] butane to give 99% n-butyraldehyde.
     alkene hydroformylation platinum diphosphine cocatalyst; alkanol
ST
     esterification platinum palladium diphosphine cocatalyst; platinum
     diphosphine carbonylation cocatalyst; palladium diphosphine carbonylation
     cocatalyst; aldehyde prepn; ester prepn
IT
     Alcohols, reactions
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (aliphatic; esterification of alkanols catalyzed by platinum or palladium
        diphosphine cocatalysts)
IT
     RL: CAT (Catalyst use); USES (Uses)
        (bidentate; carbonylation reactions of alkenes and alkanols
        catalyzed by platinum or palladium diphosphine cocatalysts)
IT
     Esterification catalysts
        (esterification of alkanols catalyzed by platinum or palladium
        diphosphine cocatalysts)
IT
     Hydroformylation catalysts
        (hydroformylation of alkenes catalyzed by platinum diphosphine
        cocatalysts)
     IT
        (hydroformylation of alkenes catalyzed by platinum diphosphine
IT
     Esterification
        (of alkanols catalyzed by platinum or palladium diphosphine
        cocatalysts)
     Hydroformylation
IT
        (of alkenes catalyzed by platinum diphosphine cocatalysts)
IT
     3375-31-3
                15170-57-7, Platinum acetylacetonate
                                                      153280-11-6
     374557-18-3
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        (carbonylation reactions of alkenes and alkanols catalyzed by platinum
       or palladium diphosphine cocatalysts)
IT
     123-72-8P, n-Butyraldehyde
                                141-32-2P
                                             590-01-2P
     RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
     (Preparation)
        (carbonylation reactions of alkenes and alkanols catalyzed by platinum
       or palladium diphosphine cocatalysts)
     71-36-3, Butanol, reactions 74-85-1, Ethene, reactions
     74-86-2, Acetylene, reactions
                                    79-09-4, Propionic acid, reactions
     115-07-1, Propene, reactions
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (carbonylation reactions of alkenes and alkanols catalyzed by platinum
       or palladium diphosphine cocatalysts)
RE.CNT
             THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
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(2) Mason, R; US---3527818 A 1970
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(4) Shell Internationale Research Maatschappij BV; WO---9505354 A 1995 HCAPLUS
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IT
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     RL: RCT (Reactant); RACT (Reactant or reagent)
        (carbonylation reactions of alkenes and alkanols catalyzed by platinum
       or palladium diphosphine cocatalysts)
RN
     3375-31-3 HCAPLUS
CN
     Acetic acid, palladium(2+) salt (8CI, 9CI) (CA INDEX NAME)
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